Decay of Electron Waves in a Random Medium

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This paper reports calculation of the time-correlation function of an electron wave of given wave vector k in a three-dimensional medium with weak scatterers randomly distributed. An initial parabolic decay is followed by the usual exponential law which, asymptotically, gives way to a $1/t^3$ law.

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An electron in a plane-wave state $\varphi_{\vec{k}}(\vec{r}, t)$ is introduced into a three-dimensional medium containing randomly situated scattering centers. The probability of its remaining in the initial state decays with time, and it is with this decay that we are concerned. While the present application is to electron waves, the method can—with suitable modifications—be applied to higher or lower dimensions, and to other type waves: phonons, magnons, etc.

A Markoffian assumption always leads to the usual exponential decay in time, with the $1/e$ lifetime τ_k given by Fermi's "golden rule":

$$1/\tau(\epsilon_k) = 2\pi g^2 \rho(\epsilon_k), \tag{1}$$

where g^2 is the mean square scattering potential and $\rho(\epsilon)$ the density of states characteristic of the unperturbed medium. However, the Markoffian assumptions are not generally justified.[1] I here undertake a more careful dynamical analysis and find that, for weak scattering, the exponential decay formula is valid only for times that are not too short nor too long compared with τ_k. Initially, the decay is parabolic, and ultimately, it is $1/t^3$.

For this analysis, I use the Green's functions of Zubarev[2] to yield the time development. The complex amplitude $A_k(t)$ of the wave is given as

$$A_k(t) \equiv \int \varphi_k^*(\vec{r}, t)\varphi_k(\vec{r}, 0)\, d^3r$$

$$= \int d\omega\, e^{i\omega t} \frac{1}{\pi} \operatorname{Im}[\omega - \epsilon_k - \Lambda_k(\omega)]^{-1}, \tag{2}$$

where $\hbar = 1$ and $\Lambda_k(\omega)$ is the (complex) correction to the particle's energy due to the scattering mechanism H'. Taking for definiteness scattering potentials of zero mean and of mean square magnitude g^2 I examine several models and limiting behavior.

For a random potential which can be $\pm g$ with equal probability, the coherent-potential approximation (CPA)[3] yields an equation

$$\Lambda(\omega) = [g^2 - \Lambda^2(\omega)] \frac{1}{N} \sum_{k'} [\omega - \epsilon_{k'} - \Lambda(\omega)]^{-1} \tag{3}$$

which has the simplifying feature that Λ does not depend on k. It has the solution

$$\Lambda(\omega) = R(\omega) + i/2\tau(\omega) \tag{4}$$

for $g^2 \to 0$. $R = O(g^2\rho(0))$ and can be neglected in the limit, whereas the imaginary part plays the decisive role in the analysis.

A variant model of a random potential, studied by Bray and Moore[4] in connection with the normal modes of a spin-glass, treats the matrix elements as constant in amplitude but random in phase, i.e.,

$$H_{kk'} = g \exp(i\theta_{k,k'}) \quad (\theta_{k,k'} = -\theta_{k',k}). \tag{5}$$

The Green's functions for this model are easily obtained by iteration, subject to a self-consistency requirement

$$\Lambda(\omega) = g^2 \frac{1}{N} \sum_{k'} [\omega - \epsilon_{k'} - \Lambda(\omega)]^{-1}; \tag{6}$$

and in the limit of weak coupling, yield precisely Eq. (4) as did the CPA. The two models differ greatly in strong coupling, however. If, for fixed g^2, we decrease the unperturbed bandwidth such that $\rho(\epsilon) = \delta(\epsilon)$, the CPA will yield $\Lambda = g^2/\omega$ whereas (6) will give $\Lambda = \frac{1}{2}\omega \pm [\frac{1}{4}\omega^2 - g^2]^{1/2}$. The former corresponds to a two-level system (poles at $\pm g$) whereas the latter reproduces Wigner's semicircular density of states of a random matrix. We shall return to the strong-coupling limits later, but start with the weak-coupling limit in which both models yield the same form of Λ, Eq. (4).

This we insert into Eq. (2), which is seen to have important contributions not only from the neighborhood of ϵ_k but, from considerations of stationary phase, at the singularities of $\rho(\omega)$ —those points at which $d\rho/d\omega$ is discontinuous.

These so-called Van Hove singularities[5] exist at the band extrema and at a number of saddle points in between. Our wave, sharp in momentum, is a wave packet in energy and those components at the Van Hove singularities will decay very slowly compared with the rest, and be responsible for the slow asymptotic decay of the prepared state.

Labeling the singularities by an index n, we have

$$A_k(t)=\left[\int_{\omega \text{ near}\epsilon_k} d\omega+\sum_n \int_{\omega \text{ near}\omega_n} d\omega\right] e^{i\omega t}\frac{g^2\rho(\omega)}{(\omega-\epsilon_k)^2+[\pi g^2\rho(\omega)]^2}=\exp(i\epsilon_k t)S_k+\sum_n \exp(i\omega_n t)\,S_n.$$

The first contribution is evidently exponential:

$$S_k=\exp(-|t|/2\tau_k) \tag{7}$$

and usually dominates. But consider the contribution from the neighborhood of the band minimum, $n=0$:

$$S_0=\frac{g^2A}{(\omega_0-\epsilon_k)^2}\int_{\omega_0}^{\omega_x} d\omega \exp[i(\omega-\omega_0)t](\omega-\omega_0)^{1/2}, \tag{8}$$

where I use the fact that in three dimensions, the density of states is $\rho=A(\omega-\omega_0)^{1/2}$ near the band minimum, and ω_x is some arbitrary cutoff. Setting $\omega-\omega_0=iy^2$ and distorting the path of integration to the real y axis, we can evaluate (8):

$$S_0=\tfrac{1}{2}i^{3/2}g^2A\pi^{1/2}(\omega_0-\epsilon_k)^{-2}t^{-3/2}. \tag{9}$$

The other singularities contribute similarly, but do not interfere if the rapidly oscillating factors $\exp(i\omega_n t)$ differ.

Thus, for times that are not too short,

$$P_k(t)=|A_k(t)|^2=\exp(-t/\tau_k)+Bt^{-3}, \tag{10}$$

where B is a constant $O(g^4)$, lumping together the contributions of all singular points and averaging over rapidly fluctuating phases. Initially, of course, (10) is not valid and so I expand in t:

$$A_k(t)=A_k(0)+\exp(i\epsilon_k t)\int d\omega[i(\omega-\epsilon_k)t-\tfrac{1}{2}(\omega-\epsilon_k)^2t^2+\ldots]\frac{g^2\rho(\omega)}{(\omega-\epsilon_k)^2+[\pi g^2\rho(\omega)]^2}, \tag{11}$$

which allows us to estimate

$$P_k(t)=1-g^2t^2+\ldots \tag{12}$$

for short times $t<\tau_k$. This demonstrates that the decay of a wave is symmetric in time, and is insensitive to any presumed "arrow of time."

While reasonable models agree in weak coupling, they yield differing results in strong coupling. We have seen that the above two models yield different Λ in strong coupling. It is easy to see that with $\rho(\epsilon)=\delta(\epsilon)$, the CPA will give $P(t)=\cos^2 gt$, whereas a straightforward calculation on the basis of Wigner's distribution yields $P(t)=[(gt)^{-1}J_1(2gt)]^2$ with J_1 the Bessel function, thus having the same parabolic initial decay and $1/t^3$ final decay as in weak coupling, without any of the exponential behavior of weak coupling. Finally, I should mention Lloyd's model,[6] in which the random potentials are distributed in strength according to a Lorentz distribution. Strictly speaking, this model has no weak-coupling limit because $\langle H'^2\rangle=\infty$, and indeed, *all* even moments higher than the second diverge. In this model $\Lambda=i\gamma$, an imaginary constant. Thus the only contribution to the integral is what we termed S_k, and the decay is precisely exponential regardless of the strength of γ. Thus we see that in strong coupling, every and any possible mode of decay is possible and there can be no general result. The reason may be that the very *concept* of a wave becomes inapplicable in strong coupling, and that a better description—perhaps in terms of Anderson's localized states[7]—may be required.

In summary, we have found that a *weak* scattering mechanism broadens a plane wave into a wave packet, in which are included states which are relatively long lived, associated with band edges and Van Hove singularities. Because of these components, the time autocorrelation function of a wave does not decay exponentially at long times, but, rather, as $1/t^3$. It is possible that these considerations may shed some light

on the more interesting problem, of the spatial autocorrelations of energy eigenstates in a disordered medium, about which there has been so much speculation lately.

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[1]With a Markoffian assumption of short-term "memory," the decay rate must be proportional to the amount of wave which remains, hence be precisely exponential. However, this assumption violates microscopic reversibility.

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Differential Cross Section for Atoms Inelastically Scattered from Surfaces

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The trajectory approximation is shown to explain the angular distribution of heavy rare-gas atoms scattered from close-packed metal surfaces, and the energy transfer for Ar on polycrystalline W. An empirical parameter, the mean energy transfer δ, is extracted.

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Energy exchange between atoms and surfaces plays a key role in phenomena such as adsorption, desorption, and accommodation. The atom-surface impact generally involves a large number of phonons. The exceptions are light atom, weak atom-surface potential V, and low surface temperature T_S, situations encountered in highly specialized He and Ne surface scattering experiments at very low temperatures. Detailed information on the scattering mechanisms in both few-phonon and multiphonon regimes is potentially contained in differential cross-section measurements in monoenergetic atomic beam scattering from single-crystal surfaces.[1-4]

It may be thought that, especially in the multiphonon regime, emphasized in this paper, these relatively complex scattering events are understandable only via detailed numerical simulations.[5] We claim below, however, success for a model more realistic than the conventional "cube" models,[6] based on the trajectory approximation (TA),[7] described shortly. From comparison with experiment, a useful energy exchange parameter for each atom/surface system can be extracted.

The trajectory approximation calculates energy and momentum transfer on the assumption that the scattering atom follows a unique classical trajectory $\vec{R}(t)$. The TA neglects surface corrugation, for which there is experimental support in the weakness of diffraction of light rare-gas atoms from close-packed metal surface,[8] making the effective atom-surface potential approximately a function $V_{\rm eff}(z)$ only of distance normal to the surface. $V_{\rm eff}$ is asymmetric, with a repulsive hard wall at small z near the surface and a long attractive tail going as z^{-3} at large z. The asymmetry of the well ensures that for high energies near the top of the well the level spacing of atoms in the well is small and can be replaced by a continuum except at very low temperatures, T, justifying a *classical* trajectory. Energy transfer to phonons occurs mostly at small z, and is normally small compared to the well depth. The insensitivity of energy or momentum trans-

